

Neutron polarization: What is it? What is it for?

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1 INTRODUCTION: THE FERMI GOLDEN RULE

In order to express the cross section of a neutron scattering process, one usually considers the probability of a transition in which the scattering system changes from $|\lambda\rangle$ to $|\lambda'\rangle$ and the neutron state changes from $|\mathbf{k}\rangle$ to $|\mathbf{k}'\rangle$, \mathbf{k} being the wave vector of the neutron. The cross section is proportional to this probability:

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\substack{\mathbf{k}\rightarrow\mathbf{k}' \\ \lambda\rightarrow\lambda'}} = \frac{k'}{k} \left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle\mathbf{k}', \lambda' | V | \mathbf{k}, \lambda\rangle|^2 \delta(E' + E_{\lambda'} - E - E_{\lambda}) \quad (1.1)$$

This expression is not fully comprehensive and should actually be replaced by a very similar expression, in which the neutron state is characterized by not only by its wave vector $|\mathbf{k}\rangle$ but also by its spin:

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\substack{\mathbf{k}\rightarrow\mathbf{k}' \\ \lambda\rightarrow\lambda' \\ \chi\rightarrow\chi'}} = \frac{k'}{k} \left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle\mathbf{k}', \lambda', \chi' | V | \mathbf{k}, \lambda, \chi\rangle|^2 \delta(E' + E_{\lambda'} - E - E_{\lambda}) \quad (1.2)$$

Indeed, the neutron carries a spin \mathbf{S} . The spin state is represented by a spin wave function $|\chi\rangle$. The neutron spins can be polarized and neutron polarization is an important aspect of neutron scattering.

2 NEUTRON SPIN AND NEUTRON POLARIZATION

2.1 The neutron carries a spin \mathbf{S}

The neutron carries a spin \mathbf{S} , which is an internal angular momentum with a quantum number $S = 1/2$. This value $S = 1/2$ means two things:

- On measuring the value taken by the operator \mathbf{S}^2 , one can only obtain a single value, its eigenvalue: $S(S+1)\hbar^2 = 3/4\hbar^2$
- On measuring the value taken by the operator S_z , the projection of the operator \mathbf{S} on the Oz axis, one finds one of its two eigenvalues: either $m_s = +1/2\hbar$, or $m_s = -1/2\hbar$, **whatever the chosen Oz axis**.

2.2 The spin wave function χ

We can define a spin wave function, a wave function in the spin space, which is a linear combination of both states:

- $|+\rangle$: S_z along Oz
- $|-\rangle$: S_z along -Oz

$$|\chi\rangle = a|+\rangle + b|-\rangle \quad (2.1)$$

with $|a|^2 + |b|^2 = 1$.

2.3 The Pauli matrices

\mathbf{S} is a vector operator: it has 3 components, represented by the 3 following matrices:

$$\begin{aligned} S_x &= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ S_y &= \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ S_z &= \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \quad (2.2)$$

In the following, we shall drop the factor $\hbar/2$ and use the operator $\boldsymbol{\sigma} = 2 \mathbf{S}/\hbar$ instead of the ‘spin operator’ \mathbf{S} . $\boldsymbol{\sigma}$ is a vector operator, the components of which are the 3 Pauli matrices:

$$\begin{aligned} \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \quad (2.3)$$

2.4 Average values and polarization

Let us start from the spin wave function of a neutron defined in Eq. 2.1:

$$|\chi\rangle = a|+\rangle + b|-\rangle$$

When one measures the value taken by the projection σ_z along Oz, one finds either +1 or -1, and no other value. If one performs the same measurements on many neutrons which have the same spin wave function 2.1 and then calculates the average of the +1 and the -1 which have been measured, one obtains the expectation value:

$$\langle \sigma_z \rangle = \langle \chi | \sigma_z | \chi \rangle \quad (2.4)$$

$$\begin{aligned} \langle \sigma_z \rangle &= \langle (a^* \langle + | + b^* \langle - |) \sigma_z (a | + \rangle + b | - \rangle) \rangle \\ \langle \sigma_z \rangle &= (a^*, b^*) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = (a^*, b^*) \begin{pmatrix} a \\ -b \end{pmatrix} \\ \langle \sigma_z \rangle &= aa^* - bb^* = |a|^2 - |b|^2 \end{aligned} \quad (2.5)$$

If the neutron is in the state $|+\rangle$, which corresponds to $a = 1$ and $b = 0$, then $\langle \sigma_z \rangle = 1$. On the contrary, if the neutron is in the state $|-\rangle$, with $a = 0$ and $b = 1$, then $\langle \sigma_z \rangle = -1$.

In the general case, when both a and b have finite values, $\langle \sigma_z \rangle = |a|^2 - |b|^2$.

Similarly, when one measures the x component of operator $\boldsymbol{\sigma}$, one finds either +1 or -1. For an ensemble of neutrons having the same spin wave function 2.1, the average of the measurements is the expectation value:

$$\begin{aligned} \langle \sigma_x \rangle &= \langle \chi | \sigma_x | \chi \rangle = \langle \chi | \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} | \chi \rangle \\ \langle \sigma_x \rangle &= a^* b + ab^* = 2 \Re(a^* b) \end{aligned} \quad (2.6)$$

and the expectation value along Oy is

$$\begin{aligned}\langle \sigma_y \rangle &= \langle \chi | \sigma_y | \chi \rangle = \langle \chi | \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} | \chi \rangle \\ \langle \sigma_y \rangle &= i(ab^* - a^*b) = 2 \Im(a^*b)\end{aligned}\quad (2.7)$$

The 3 quantities $\langle \sigma_x \rangle$, $\langle \sigma_y \rangle$ and $\langle \sigma_z \rangle$ are the 3 components of the vector \mathbf{p} , ‘polarization of the neutron’:

$$\mathbf{p} \begin{cases} p_x = \langle \sigma_x \rangle \\ p_y = \langle \sigma_y \rangle \\ p_z = \langle \sigma_z \rangle \end{cases} \quad (2.8)$$

Note: The spin operator \mathbf{S} , as well as the ‘Pauli matrices’ operator $\boldsymbol{\sigma} = 2 \mathbf{S}/\hbar$ are quantum vector operators and it is not possible to have a complete knowledge of their 3 components. On the other hand, **the polarization \mathbf{p} is a classical vector** as it is built from the three expectation values. It is therefore possible to:

- measure simultaneously its 3 components
- control its rotation in the 3-dimensional space

2.5 Examples of neutron spin wave function and neutron polarization

Let us take the example of a spin wave function $|\chi\rangle = \frac{1}{\sqrt{2}}[|+\rangle + |-\rangle]$. As $a = b = \frac{1}{\sqrt{2}}$, we have :

$$\begin{aligned}\langle \sigma_x \rangle &= \langle \chi | \sigma_x | \chi \rangle = ab^* + a^*b = 1 \\ \langle \sigma_y \rangle &= \langle \chi | \sigma_y | \chi \rangle = i(ab^* - a^*b) = 0 \\ \langle \sigma_z \rangle &= \langle \chi | \sigma_z | \chi \rangle = |a|^2 - |b|^2 = 0\end{aligned}$$

When measuring the σ_z component of an ensemble of neutrons having the above spin wave function, one obtains sometimes +1 and sometimes -1, but the average is zero. When measuring the σ_y component of this ensemble of neutrons, one finds sometimes +1 and sometimes -1, the average is also zero. But, when measuring the σ_x component of the same ensemble of neutrons, one always obtains +1. These neutrons are polarized along Ox .

Similarly, with a spin wave function $|\chi\rangle = \frac{1}{\sqrt{2}}[|+\rangle - |-\rangle]$, the polarization is along $-Ox$.

With a spin wave function: $|\chi\rangle = \frac{1}{\sqrt{2}}[|+\rangle + i|-\rangle]$, the polarization is along Oy .

With a spin wave function: $|\chi\rangle = \frac{1}{\sqrt{2}}[|+\rangle - i|-\rangle]$, the polarization is along $-Oy$.

Note: From the above examples, one can see in the expression of the spin wave functions that the phase between $|+\rangle$ and $|-\rangle$ determines the direction of the polarization in the xy plane.

2.6 Polarization of a neutron beam

In a neutron beam the individual polarizations of the neutrons may differ from each other. One can define the polarization of the beam as the average of the individual polarizations of all the neutrons of the beam:

$$\mathbf{P} = \frac{1}{N} \sum_j \mathbf{p}_j \quad (2.9)$$

with, obviously:

$$0 \leq |\mathbf{P}| \leq 1 \quad (2.10)$$

3 NEUTRON SPIN AND NEUTRON MAGNETIC MOMENT

3.1 The neutron carries a magnetic moment

The neutron carries a magnetic moment and this moment is related to the spin:

$$\boldsymbol{\mu}_n = \gamma_L \langle \mathbf{S} \rangle \quad (3.1)$$

For the neutron, the gyromagnetic ratio γ_L is negative, which means that the magnetic moment is opposed to the spin angular momentum.

3.2 Action of a magnetic field

A magnetic field exerts a torque on the neutron moment, as it does on any magnetic moment:

$$\boldsymbol{\Gamma} = \boldsymbol{\mu}_n \times \mathbf{B} = \gamma_L \langle \mathbf{S} \rangle \times \mathbf{B} \quad (3.2)$$

Magnetic fields are therefore the tools which are used to control the neutron polarization.

In a steady magnetic field: the Larmor precession

Let us compare the action of a steady magnetic field on the neutron magnetic moment to the effect of the gravitation field on a spinning top. The gravity field exerts a strength, the weight w , on the center of gravity of the top (see Figure 1), which leads to a torque:

$$\boldsymbol{\Gamma} = \mathbf{OG} \times \mathbf{w}$$

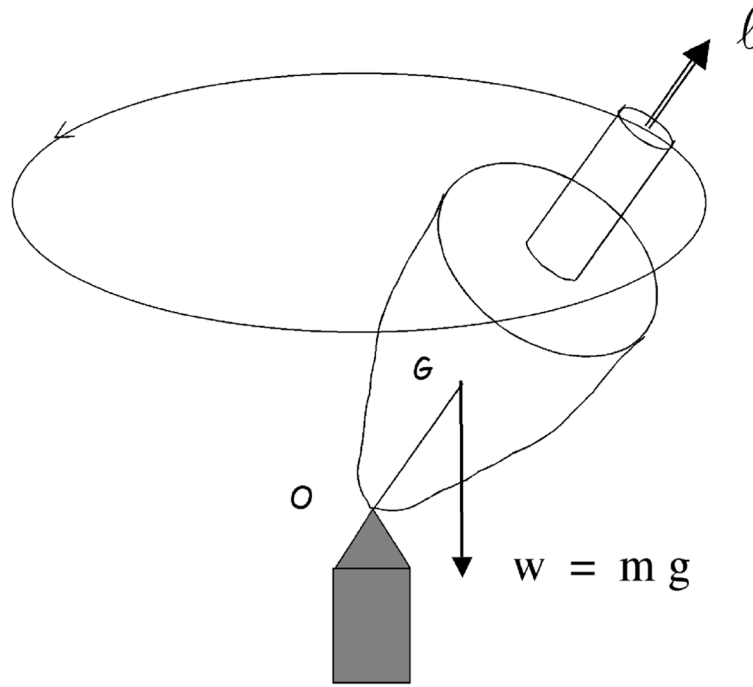


Figure 1. The angular momentum of a spinning top rotating around the gravitation axis.

If the top is not spinning, this torque will make the top fall; but if the torque is spinning, the axis of the top (the angular momentum ℓ) will rotate around the vertical axis, the direction of the gravitation field.

Similarly, in a steady magnetic field B , a torque is exerted on the magnetic moment of the neutron (formula 3.2), and this moment (as well the polarization) will rotate around the magnetic field.

The corresponding pulsation (Larmor pulsation) is given by:

$$\omega_L = \gamma_L B \quad (3.3)$$

which corresponds to a very fast rotation: over 3000 turns/sec in a 1 gauss field and 10^4 times faster in a 1 tesla field.

In a varying magnetic field

The polarization keeps rotating around the field B with a Larmor frequency $2\pi\omega_L$. What happens then if the field varies along the neutron path? We can consider two extreme cases:

- **If the field varies slowly compared to the Larmor frequency**, the neutron polarization experiences many turns around the field before the field really changes direction. The neutron polarization does not feel that the field changes and follows the field during its rotation. Such a rotation of the polarization is called ‘adiabatic’.
- **If the field changes very suddenly compared to the Larmor frequency**, the neutron polarization has no time to react when the field direction changes: it was rotating around B_1 and then, suddenly, much faster than a Larmor period, B_1 becomes B_2 . Surprised, the neutron polarization stops rotating around B_1 which does not exist anymore and starts rotating around B_2 .

In the intermediate cases, when the rate of change of the field ω_B is of the same order of magnitude as the Larmor pulsation, the rotation of the polarization is partial and depends on the adiabaticity parameter ω_L/ω_B .

Guide fields

In practice, once the neutrons have been polarized by a polarizing device, any field along their path through the experimental set up (stray field, earth field) is able to rotate their polarization in an uncontrolled way. To prevent such troubles, guide fields are installed all along the neutron paths to guide this polarization. The neutron polarization rotates around these fields. If parasitic fields are present, they will slightly twist the guide fields, but the neutron polarization will follow the guide fields, these guide fields playing the role of polarization controllers.

4 POLARIZED NEUTRON SCATTERING

4.1 Polarized neutrons without polarization analysis [1,2]

Description of the set-up

In such a simple polarized neutron diffractometer, the incident neutrons are polarized but the polarization of the scattered neutrons is not analyzed.

A vertical magnetic field magnetizes the monochromator which plays a double role: selecting neutrons with the same wavelength, but also polarizing their spins. Then, the polarization of the incident beam can be reversed by a flipping device inserted between the monochromator and the sample, allowing the polarization to be either ‘up’ or ‘down’ when arriving on the sample. And, finally, another magnetic field magnetizes the sample.

Vertical guide fields are present between the monochromator and the sample in order to keep the polarization vertical, whether the spin flipper is activated or not.

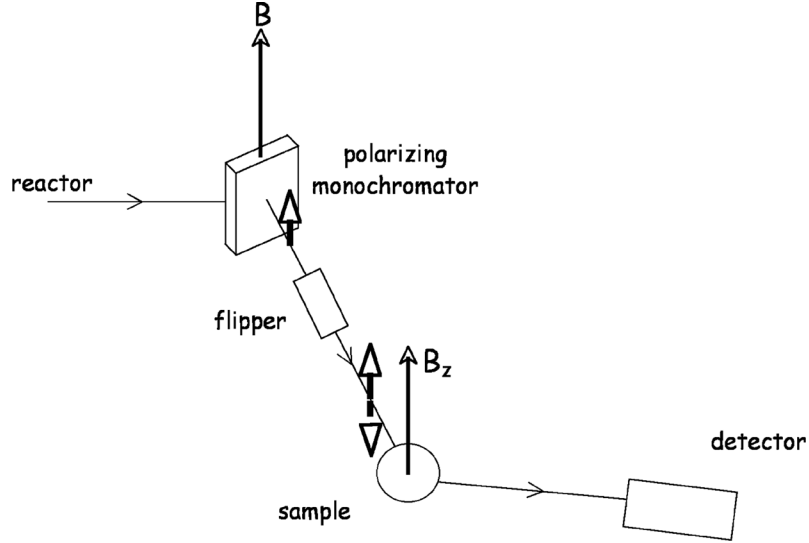


Figure 2. Diagram of a polarized neutron diffraction experiment.

For each Bragg reflection, the experiment consists in a double measurement of the scattered intensities: one with the polarization of the incident beam parallel to the magnetization of the sample (I^+), and one with the beam polarization reversed (I^-).

Enhancement of the sensitivity

For a Bragg reflection due to both nuclear scattering (nuclear amplitude N) and magnetic scattering (magnetic amplitude M), if the neutrons are not polarized, one measures an intensity which is the sum of the nuclear and the magnetic intensities ¹:

$$I = N^2 + M^2 \quad (4.1)$$

For the same Bragg reflection, if the incoming neutrons are polarized in the + (or -) direction, one measures an intensity which is essentially the square of the sum (or the difference) of the nuclear and the magnetic amplitudes:

$$I^\pm = (N \pm M)^2 = N^2 + M^2 \pm 2NM \quad (4.2)$$

This represents a tremendous enhancement of the sensitivity for the measurement of the small magnetic amplitudes. To illustrate this difference, let us take an example where the magnetic amplitude is 10% of the nuclear one ($M = 0.1N$). For non polarized neutrons, the magnetic intensity represents 1% of the nuclear intensity ($N^2 + M^2 = 1 + 0.01$). For polarized neutrons, the magnetic intensity represents around 20% of the nuclear one ($N^2 + M^2 \pm 2NM = 1 + 0.01 \pm 0.20$). This enhancement of sensitivity is due to the double product NM where the nuclear amplitudes play the role of amplifiers for the measurements of the magnetic ones.

Therefore, polarized neutrons without polarization analysis, make it possible to measure small magnetic amplitudes, and particularly magnetic amplitudes which are far in the reciprocal space. They are the ideal tool to measure magnetic form factors and spin (or magnetization) distributions.

¹The formula is only approximate: for simplicity we have written squares instead of modulus squared

Chirality

Eq. 4.2 above is incomplete as one term has been omitted. A more correct expression is:

$$I^{\pm} = N^2 + M^2 \pm 2[NM_z + i(\mathbf{M}^* \times \mathbf{M})_z] \quad (4.3)$$

where Oz is the direction of the incoming polarization. This formula includes the chiral contribution $i(\mathbf{M}^* \times \mathbf{M})_z$, a term which disappears if the neutrons are not polarized.

Where does such a term come from? Let us decompose the magnetic amplitude vector \mathbf{M} into its real and its imaginary parts:

$$\mathbf{M} = \mathbf{A} + i\mathbf{B}$$

$$\mathbf{M}^* = \mathbf{A} - i\mathbf{B}$$

then

$$i(\mathbf{M}^* \times \mathbf{M}) = 2\mathbf{B} \times \mathbf{A}$$

A magnetic structure is chiral if it is different from its image in a mirror (as a right or a left hand). Then \mathbf{M} is not parallel to \mathbf{M}^* , or, what is equivalent, if \mathbf{A} is not parallel to \mathbf{B} . Let us recall here that \mathbf{M} is a vector magnetic amplitude or, in other words the vector magnetic structure factor.

The simplest example of chiral structure with one atom per unit cell is a simple helix for which $\mathbf{M} = \mathbf{u} + i\mathbf{v}$. But, more generally, a magnetic structure with several non collinear magnetic moments per cell has magnetic structure factors which are complex and not parallel to their conjugates. Such a structure is chiral and this chirality can be analyzed with polarized neutrons.

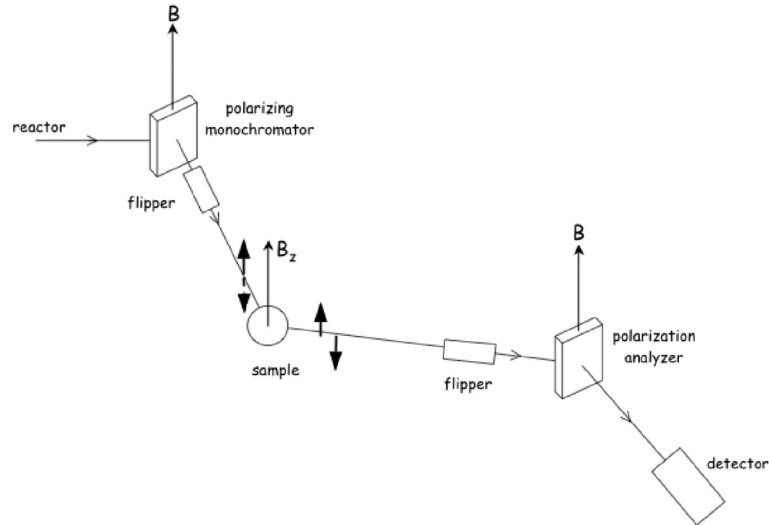


Figure 3. Experimental arrangement for the uniaxial polarization analysis [3].

4.2 Uniaxial (longitudinal) polarization analysis [3]

Description of the experiments

A new field of investigation has been opened when Moon et al.[3] showed that it is possible to analyze the scattered polarization by adding a polarization analyzer after the sample.

In this first method of polarization analysis, the incoming neutrons are polarized in a given direction of space and the polarization of the scattered neutrons is analyzed **in the same direction of space** (see Figure 3). This polarization analysis method is therefore called **uniaxial** polarization analysis. Sometimes, the designation ‘longitudinal polarization analysis’ is used instead of ‘uniaxial polarization analysis’.

The 4 partial intensities (cross sections)

Introducing also a second spin flipper between the sample and the analyzer, one can select not only the + or – direction for the incoming polarization, but also the + or – direction for the scattered polarization. It is therefore possible to measure 4 partial intensities (cross sections) corresponding to the different combinations²:

$$I^{++} \propto \sigma^{++} = (N + M_z)^2 \quad (4.4)$$

$$I^{--} \propto \sigma^{--} = (N - M_z)^2 \quad (4.5)$$

$$I^{+-} \propto \sigma^{+-} = (M_x + iM_y)^2 \quad (4.6)$$

$$I^{-+} \propto \sigma^{-+} = (M_x - iM_y)^2 \quad (4.7)$$

The 2 partial cross sections σ^{++} and σ^{--} correspond to situations where the spin of the neutrons remains the same during the scattering process; they are called the ‘non spin-flip’ cross sections. They refer to the nuclear amplitude and the magnetic component which is parallel to the polarization. On the contrary, σ^{+-} and σ^{-+} are the ‘spin-flip’ cross sections and represent a scattering due solely to the magnetic components which are perpendicular to the polarization.

As will be developed in the further lectures, uniaxial polarization analysis is the fundamental tool to separate magnetic from nuclear scattering when both scatterings occur in the same portion of the reciprocal space.

Uniaxial polarization analysis: the XZ method

Formulae (4.4 - 4.7) are incomplete in that sense that they do not take into account the incoherent scattering (isotope incoherent NN_{incoh} and nuclear spin incoherent SS_{incoh}). Introducing their contributions, the complete formulae are:

$$\sigma^{++} = (N + M_z)^2 + \frac{1}{3}SS_{incoh} + NN_{incoh} \quad (4.8)$$

$$\sigma^{--} = (N - M_z)^2 + \frac{1}{3}SS_{incoh} + NN_{incoh} \quad (4.9)$$

$$\sigma^{+-} = (M_x + iM_y)^2 + \frac{2}{3}SS_{incoh} \quad (4.10)$$

$$\sigma^{-+} = (M_x - iM_y)^2 + \frac{2}{3}SS_{incoh} \quad (4.11)$$

Therefore, in order to disentangle the nuclear from the magnetic cross sections, instead of comparing spin flip and non spin flip scattering, it is generally more accurate to compare either the ‘spin flip’ or the ‘non spin flip’ scattering for two different settings of the uniaxial polarization: polarization vertical (direction \mathbf{Z}) and polarization along the scattering vector (direction \mathbf{X}). The difference between the two measurements gives directly the coherent magnetic contribution, all the incoherent contributions vanishing in the difference (see Figure 4).

$$(\sigma^{++})_{\mathbf{P} // \mathbf{Z}} - (\sigma^{++})_{\mathbf{P} // \mathbf{X} = \mathbf{Q}} = |M_z|^2 \quad (4.12)$$

$$(\sigma^{+-})_{\mathbf{P} // \mathbf{X} = \mathbf{Q}} - (\sigma^{+-})_{\mathbf{P} // \mathbf{Z}} = |M_z|^2 \quad (4.13)$$

This fruitful comparison may be achieved on the spin flip as well as on the non spin flip scattering patterns. The result is formally the same. The choice between these two spin configurations will depend on the amount of incoherent scattering for each case, incoherent scattering which eliminates in the difference but which increases the error bars.

²Here also, for simplicity, we have written squares instead of moduli squared

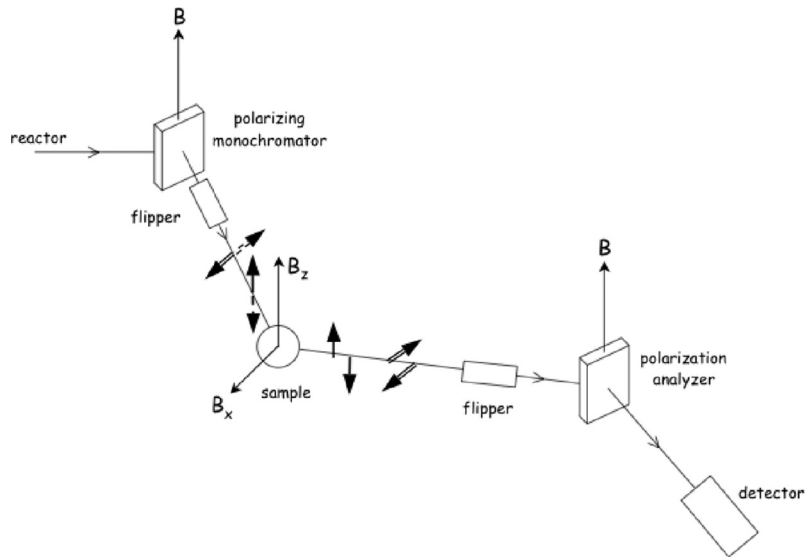


Figure 4. Scheme of the experimental arrangement for the XZ method in the uniaxial polarization analysis.

Three-dimensional uniaxial polarization analysis [4]

Formulae 4.12 and 4.13 imply that one of the measurements is performed with the uniaxial polarization along the scattering vector. In some cases, it is not possible to align the polarization along the scattering vector:

- in the case of elastic scattering with multidetectors which collect at the same time neutrons corresponding to different scattering vectors
- in the case of inelastic scattering when a detector collects neutrons having the same diffused wave vector \mathbf{k} , but corresponding to different scattering vectors \mathbf{Q}

The XYZ method has been implemented for such cases [4]. In this method, either for the spin flip scattering, or for the non spin flip scattering, the differences concern now three different diagrams: one with the uniaxial polarization vertical (direction \mathbf{Z}) and the other two with the uniaxial polarization along two orthogonal directions in the horizontal plane (directions \mathbf{X} and \mathbf{Y}), as shown in Figure 5. Neither X nor Y is in the direction of the scattering vector (direction which is no more unique). However, the two formulae 4.12 and 4.13 can be applied practically as they are (to within one coefficient), at the condition that an average diagram between the two diagrams with $\mathbf{P} // \mathbf{X}$ and $\mathbf{P} // \mathbf{Y}$ replaces the diagram with $\mathbf{P} // \mathbf{Q}$. To achieve such measurements, the polarization is turned by a system of guide fields. In particular, the field on the sample is provided by a triple Helmholtz coil, one coil oriented along \mathbf{X} , one along \mathbf{Y} and one along \mathbf{Z} .

It is important to note that this XYZ method, though being tridimensional, is nevertheless uniaxial as, for each measurement, the direction of analysis of the scattered polarization is the same as the polarization of the incident beam. A magnetic field is applied on the sample: the incident polarization is parallel to it and only the component of the scattered polarization parallel to this field is analyzed.

Spherical polarization analysis [5]

In this concept, for each direction of the incident beam polarization, the polarization of the scattered beam is analyzed in the 3 dimension of space. Formally, this means that for each of the 3 directions \mathbf{X} , \mathbf{Y} or \mathbf{Z} of the incident polarization, one measures the 3 components of the scattered polarization. This represents 9 measurements (see Figure 6).

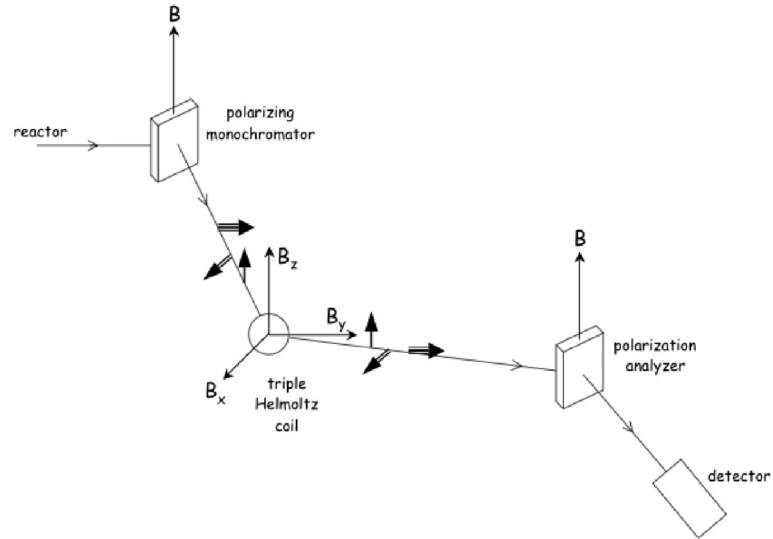


Figure 5. Scheme of the tridimensional uniaxial polarization analysis.

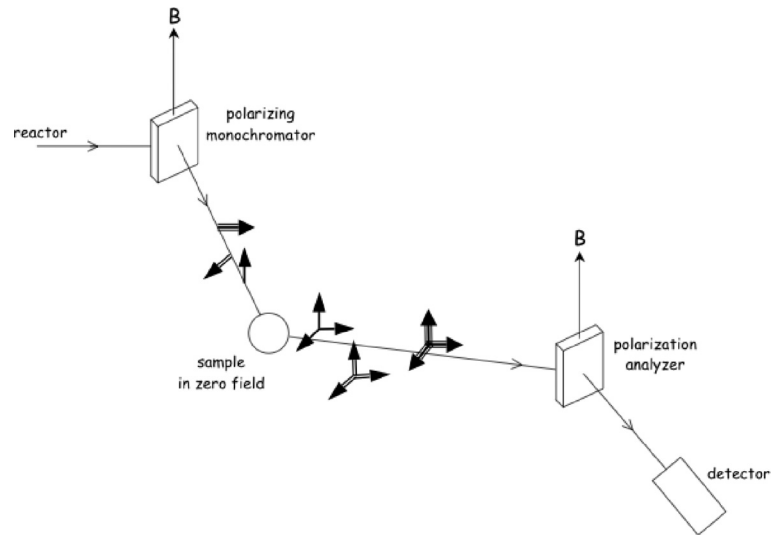


Figure 6. Scheme of a spherical polarization analysis setup [5].

The scattered polarization may be written as:

$$\mathbf{P}' = \mathbf{P}'_0 + \overline{\overline{T}} \mathbf{P} \quad (4.14)$$

where the first part \mathbf{P}'_0 is a polarization which is created during the scattering, and where the second part $\overline{\overline{T}} \mathbf{P}$ represents a rotation of the incident polarization during the scattering. $\overline{\overline{T}}$ is a 3x3 tensor.

The 3 components of the vector \mathbf{P}'_0 may be directly determined by the measurement of the 3 components of the scattered polarization with an incident beam which is not polarized. The 9 elements of tensor $\overline{\overline{T}}$ are determined from the 9 polarimetry measurements of polarized beams, as explained above.

It is important to note that in this technique, for each direction of the incident polarization, the direction of the scattered polarization is analyzed in the 3 directions of space. It is important that this scattered polarization is not perturbed by a magnetic field on the sample. Therefore, in this technique, no magnetic field is present around the sample.

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